

## Non-Abelian Bosonization and Haldane's Conjecture

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### Abstract

We study the long wavelength limit of a spin  $S$  Heisenberg antiferromagnetic chain. The fermionic Lagrangian obtained corresponds to a perturbed level  $2S$   $SU(2)$  Wess-Zumino-Witten model. This effective theory is then mapped into a compact  $U(1)$  boson interacting with  $Z_{2S}$  parafermions. The analysis of this effective theory allows us to show that when  $S$  is an integer there is a mass gap to all excitations, whereas this gap vanishes in the half-odd-integer spin case. This gives a field theory treatment of the so-called Haldane's conjecture for arbitrary values of the spin  $S$ .

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In 1983 Haldane conjectured that in the case of integer spin, the spin  $S$  quantum Heisenberg Antiferromagnetic (HAF) chain has a unique disordered ground state with a finite excitation gap, while the same model has no excitation gap when  $S$  is a half-odd-integer [1]. Using a mapping to the non-linear  $\sigma$  Model, valid in the large  $S$  limit, the origin of the difference has been identified as being due to an extra topological “ $\Theta$  term” in the effective  $\sigma$ -model Lagrangian for systems with half-integer  $S$  [1]. This clearly suggests that the origin of this difference is non-perturbative. Although Haldane’s predictions were based on large- $S$  arguments, it is known that this conjecture is consistent with the Bethe Ansatz exact solution which is available for  $S = 1/2$  [2], and experimental, numerical, and theoretical studies almost confirmed its validity for  $S = 1$  [3]. For higher half-odd-integer spin the ground state is either degenerate or has a massless excitation [4] which suggests but does not prove critical correlations. In [5] massless behavior in  $S = 3/2$  has been tested numerically (see also [6]). Recent experimental evidence of the existence of the Haldane gap for  $S = 2$  HAF chains has been found in the study of the compound  $MnCl_3(bipy)$  [7].

Bosonization techniques have been extensively used in the study of spin chains (see [8] for a review on the subject and references therein). The starting point consists on the mapping of the original problem, in terms of spin variables, to the problem of fermionic variables with additional constraints (which are necessary for the two systems to be equivalent) and then bosonize the resulting system. In [9], the HAF model was formulated as a certain limit of the Hubbard model. By using a bosonization technique and a renormalization group analysis, they found an effective theory for the low-energy physics of  $S = 1/2$  and the limit of large  $S$  spin chains. In [10] another approach was used which relies on the fact that the spin  $S$  HAF chain can be represented as  $2S$  spin  $1/2$  chains for large ferromagnetic coupling. In a recent paper [11] the issue of implementing explicitly the above mentioned additional constraints within the path-integral approach was taken up, and a reconfirmation of Haldane’s conjecture was obtained for large values of the spin  $S$ , by using non-abelian bosonization techniques.

In this Letter we study the effective low energy theory in terms of a fermionic coset model which corresponds to the level  $2S$   $SU(2)$  Wess-Zumino-Witten (WZW) theory [12,13] following [11], and map it into a coupled system of a compact  $U(1)$  boson and  $Z_{2S}$ -Parafermions (PF). The analysis of the phase diagrams of  $Z_{2S}$  models together with the knowledge of their operator product algebra provide us with the elements to establish the difference between integer and half-integer spin chains.

We would like to stress that our analysis does not rely on a large  $S$  approximation, but is valid for all values of  $S$ .

Let us briefly review the work of [11]: The spin  $S$  HAF model can be written in terms of fermionic operators  $C_{\alpha ix}$ , with  $\alpha = \uparrow, \downarrow; i = 1, \dots, 2S$ .  $\alpha$ ,  $i$  and  $x$  are spin, color and site indices, respectively. The spin  $S$  operator on one site  $x$  is represented by

$$\vec{S}_x = C_{\alpha ix}^\dagger \frac{\vec{\sigma}_{\alpha\beta}}{2} C_{\beta ix}, \quad (1)$$

where  $\vec{\sigma}_{\alpha\beta}$  are the Pauli matrices. In order to correctly represent the spin  $S$  chain, the physical states must satisfy

$$\sum_i C_{\alpha ix}^\dagger C_{\alpha ix} |phys\rangle = 2S |phys\rangle$$

$$\sum_{ij} C_{\alpha ix}^\dagger \tau_{ij}^a C_{\alpha jy} |phys\rangle = 0, \quad (2)$$

where  $\tau^a$  are the  $SU(2S)$  generators. The first constraint imposes the condition that allows only one spin per site, whereas the second one states that the physical states must be color singlets.

The Heisenberg Hamiltonian

$$H = \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y \quad (3)$$

can be expressed in terms of the fermionic operators introduced above as

$$H = -\frac{1}{2} \sum_{\langle xy \rangle} C_{\alpha ix}^\dagger C_{\alpha jy} C_{\beta jy}^\dagger C_{\beta ix} + \text{constant}. \quad (4)$$

which has a local  $SU(2S) \times U(1)$  invariance. This quartic interaction can be rewritten by introducing an auxiliary field  $B$  as

$$H = \frac{1}{2} \sum_{\langle xy \rangle} (B_{xy}^{ij} C_{\alpha ix}^\dagger C_{\alpha jy} + h.c. + \bar{B}_{yx}^{ji} B_{xy}^{ij}). \quad (5)$$

In the mean field approximation  $B$  is a constant  $2S \times 2S$  matrix, and  $H$  can be diagonalized. To obtain an effective low energy theory we keep the operators  $C(k)$  with  $k$  near the Fermi surface  $\pm\pi/2a$ . We can then write

$$\frac{1}{\sqrt{a}} C_{\alpha ix} = e^{\frac{i\pi}{2a}x} \Psi_{R\alpha i}(x) + e^{-\frac{i\pi}{2a}x} \Psi_{L\alpha i}(x), \quad (6)$$

where  $\frac{1}{\sqrt{a}}$  appears for dimensional reasons and  $\Psi_{R,L\alpha i}(x)$  are slowly varying on the lattice scale.

We also expand the field  $B$  as

$$B_{xy} = B_0 e^{aV_{xy}} \simeq B_0 (1 + aV_{xy}), \quad (7)$$

and define  $A_1 \equiv \frac{1}{2}(V_{xy} - V_{xy}^\dagger)$  and  $R_{xy} \equiv \frac{1}{2}(V_{xy} + V_{xy}^\dagger)$ . When substituted back into the Hamiltonian, the expansion (7) leads to a quadratic integral in  $R_{xy}$  which can be performed to give

$$H = B_0 \left( -i\Psi_{Ri}^\dagger (\delta_{ij} \partial_x + A_{ij}^1) \Psi_{Rj} + i\Psi_{Li}^\dagger (\delta_{ij} \partial_x + A_{ij}^1) \Psi_{Lj} \right) + \frac{1}{4} \left( \Psi_{Li}^\dagger \Psi_{Rj} - \Psi_{Ri}^\dagger \Psi_{Lj} \right)^2, \quad (8)$$

The effective Lagrangian is obtained by introducing a Lagrange multiplier  $A_0$  in the Lie algebra of  $U(2S)$ , together with the use of the identity

$$\delta[\bar{\Psi}_i \Psi_j] = \lim_{\lambda_2 \rightarrow \infty} e^{-\lambda_2 \int d^2x (\bar{\Psi}_i \Psi_j)^2}, \quad (9)$$

in order to implement the constraints (2) (see [11] for details). The effective Lagrangian then reads

$$L = \bar{\Psi} \gamma^\mu i D_\mu \Psi - \lambda_1 (i \bar{\Psi}_i \gamma_5 \Psi_j)^2 - \lambda_2 (i \bar{\Psi}_i \Psi_j)^2, \quad (10)$$

where  $D_\mu = \partial_\mu - i a_\mu + B_\mu$ , and we have decomposed, for later convenience, the field  $A_\mu$  into a  $U(1)$  field  $a_\mu$  and a  $SU(2S)$  field  $B_\mu$ .

The Lagrangian can be rewritten as

$$\begin{aligned} L = & \bar{\Psi}_{i\alpha} \gamma^\mu i (\partial_\mu - i a_\mu \delta_{ij} \delta_{\alpha\beta} + B_\mu^{ij} \delta_{\alpha\beta}) \Psi_{j\beta} + \\ & + 4(\lambda_1 + \lambda_2) \vec{J}_{R\cdot} \vec{J}_L + (\lambda_1 + \lambda_2) j_R j_L + \\ & - (\lambda_1 - \lambda_2) (\Psi_{Ri\alpha}^\dagger \Psi_{Lj\alpha} \Psi_{Rj\beta}^\dagger \Psi_{Li\beta} + h.c.), \end{aligned} \quad (11)$$

where  $\vec{J}_{R,L} = \Psi_{R,Li\alpha}^\dagger \frac{\vec{\sigma}_{\alpha\beta}}{2} \Psi_{R,Li\beta}$ ,  $j_{R,L} = i \Psi_{R,Li\alpha}^\dagger \Psi_{R,Li\alpha}$  are  $SU(2)_{2S}$  and  $U(1)$  currents respectively.

The first term in the Lagrangian (11) corresponds to the fermionic coset version of the level  $2S$   $SU(2)$  WZW theory [14] as was already observed in [11]. In this context the original spin operator corresponds to the fundamental field of the WZW model. The third term can be absorbed by a redefinition of the  $U(1)$  gauge field  $a_\mu$ .

Thus, we have to deal with the second and last terms in (11) which can be expressed as

$$\Delta \mathcal{L} = (\lambda_1 - \lambda_2) (g_{\alpha\beta} g_{\beta\alpha} + h.c.) + 4(\lambda_1 + \lambda_2) \vec{J}_{R\cdot} \vec{J}_L \quad (12)$$

where  $g \equiv \Psi_{Ri}^\dagger \Psi_{Li}$  is the spin 1/2 primary field of the  $SU(2)_{2S}$  WZW theory,  $\Phi^{(1/2)}$ , with conformal dimensions  $h = \bar{h} = 3/(8(S+1))$ . The first term in (12) corresponds to the spin 1 affine primary  $\Phi^{(1)}$  with conformal dimensions  $h = \bar{h} = 1/(S+1)$ , so we can write

$$\Delta \mathcal{L} = -4 (\lambda_1 - \lambda_2) \text{tr} \Phi^{(1)} + 4(\lambda_1 + \lambda_2) \vec{J}_{R\cdot} \vec{J}_L \quad (13)$$

The  $S = \frac{1}{2}$  case is simpler, as has been discussed in [9], [11], since affine (Kac-Moody) selection rules forbid the appearance of the relevant operator  $\Phi^{(1)}$ . We then have an effective massless theory in accordance with Haldane's predictions. The second term in (13) is marginally irrelevant since  $\lambda_1 + \lambda_2$  is positive, and gives the well-known logarithmic corrections to correlators.

For higher spins, we have to consider the interaction term (13) and we also have to include all other terms which will be radiatively generated. We then need the operator product expansion (OPE) coefficients among the different components of  $\Phi^{(1)}$  which have been computed in [15]. The OPE coefficients are non-vanishing iff the so called ‘‘Fusion Rules’’ are non-vanishing. In the level  $k$   $SU(2)$  WZW theory they are given by [16]

$$\Phi_{m,\bar{m}}^{(j)} \times \Phi_{m',\bar{m}'}^{(j')} = \sum_{n=|j-j'|}^{\min(j+j', k-j-j')} \Phi_{m+m', \bar{m}+\bar{m}'}^{(n)} \quad (14)$$

We will use that [15,17]

$$SU(2)_k \equiv Z_k \otimes U(1) \quad (15)$$

in the sense that the Hilbert spaces of the two theories coincide. We will exploit this equivalence to derive an effective low energy action for the spin  $S$  HAF chain. Indeed, it

was shown in [15] that the primary fields of the  $SU(2)_k$  WZW theory are related to the primaries of the  $Z_k$ -parafermion theory and the  $U(1)$  vertex operators. They are connected by the relation

$$\Phi_{m,\bar{m}}^{(j)}(z, \bar{z}) = \phi_{2m,2\bar{m}}^{(2j)}(z, \bar{z}) : e^{\frac{i}{\sqrt{2S}}(m\varphi(z) + \bar{m}\bar{\varphi}(\bar{z}))} :, \quad (16)$$

where the  $\Phi$  fields are the invariant fields of the  $SU(2)_k$  WZW theory, the  $\phi$  fields are the  $Z_k$  PF primaries and  $\varphi$  and  $\bar{\varphi}$  are the holomorphic and antiholomorphic components of a compact massless free boson field. In the same way, the currents are related as

$$\begin{aligned} J_R^+(z) &= (2S)^{1/2} \psi_1(z) : \exp\left(\frac{i}{\sqrt{2S}}\varphi(z)\right) : , \\ J_R^0(z) &= (2S)^{1/2} \partial_z \varphi(z) \end{aligned} \quad (17)$$

where  $\psi_1$  is the first parafermionic field. (A similar relation holds for the left-handed currents).

Using this equivalence we can express the relevant perturbation term (13) as

$$\begin{aligned} \Delta\mathcal{L} &= -4(\lambda_1 - \lambda_2) \left( \phi_{0,0}^{(2)} + \phi_{2,-2}^{(2)} : e^{\frac{i}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : \right. \\ &\quad \left. + \phi_{-2,2}^{(2)} : e^{-\frac{i}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : \right) \\ &\quad + 4S(\lambda_1 + \lambda_2) \left( \psi_1 \bar{\psi}_1^\dagger : e^{\frac{i}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c. \right), \end{aligned} \quad (18)$$

where we absorbed the derivative part of the  $U(1)$  field coming from (17) into a redefinition of the constant in front of the unperturbed Lagrangian. The first term corresponds to the first “thermal” field of the PF theory,  $\phi_{0,0}^{(2)} = \epsilon_1$ , with conformal dimensions  $h = \bar{h} = 1/(1 + S)$ , while the second and third terms correspond to the  $p = 2$  disorder operator in the PF theory,  $\phi_{2,-2}^{(2)} = \mu_2$  and its adjoint  $\phi_{-2,2}^{(2)} = \mu_2^\dagger$  with dimensions  $d_2 = \bar{d}_2 = (S - 1)/(2S(S + 1))$ .

Including all the operators which are radiatively generated we get three “families” of perturbations:

- 1) The thermal operator  $\epsilon_1$  and all the members of its sub-algebra (higher thermal operators). As shown in [18], the  $Z_{2S}$  PF theory perturbed by  $\epsilon_1$  flows into a massive regime, irrespectively of the sign of the coupling. Assuming that, as for the  $Z_2$  case, due to the sign of the coupling  $\lambda_1 - \lambda_2$  in (18) the theory is driven into a low temperature ordered phase, we have that vacuum expectation values (v.e.v.’s) of disorder operators  $\mu_j$ , vanish for  $j \neq 2S \bmod(2S)$  as well as v.e.v.’s of the parafermionic fields  $\langle \psi_k \bar{\psi}_k^\dagger \rangle = 0$ , for  $2k \neq 2S \bmod(2S)$ .
- 2) The family of the disorder operator (with the corresponding vertex operators) given by:

$$\sum_{k=1}^{[S]} \mu_{2k} : e^{\frac{ik}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c.$$

where  $[S]$  means integer part of  $S$ . Note that  $\mu_{2S}$  corresponds to the identity operator and then for  $S$  integer, this family contains the single vertex operator

$$: e^{\frac{iS}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c. \quad (19)$$

3) The family of the parafermionic fields:

$$\sum_{k=1}^{2S} \psi_k(z) \bar{\psi}_k^\dagger(\bar{z}) : e^{\frac{ik}{\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c.$$

Note that the system is invariant under the extended  $Z_{2S} \times \tilde{Z}_{2S}$  transformation

$$\begin{aligned} \mu_p &\rightarrow w^{p(m-n)} \mu_p ; \quad \psi_p \bar{\psi}_p^\dagger \rightarrow w^{2p(m-n)} \psi_p \bar{\psi}_p^\dagger ; \\ \varphi &\rightarrow \varphi - \frac{\sqrt{2}\pi m}{\sqrt{S}} ; \quad \bar{\varphi} \rightarrow \bar{\varphi} - \frac{\sqrt{2}\pi n}{\sqrt{S}} \end{aligned} \quad (20)$$

with  $w = \exp(\pi i/S)$  and  $m, n \in \mathbb{Z}$ .

Since the parafermionic sector is massive, the effective theory for large scales can be obtained by integrating out these degrees of freedom. Since this massive sector is driven into the phase where (20) is unbroken, we can obtain the most general effective action for the remaining  $U(1)$  field, where only the vertex operators invariant under (20) will be allowed to appear. We get

$$\begin{aligned} Z_{eff} &= \int \mathcal{D}\phi \exp \left( - \int K_S (\partial_\mu \phi)^2 + \right. \\ &\quad \left. \alpha_S \int \cos\left(\frac{2S}{\sqrt{2S}}(\varphi - \bar{\varphi})\right) + \dots \right), \end{aligned} \quad (21)$$

for  $S$  half-integer, and

$$\begin{aligned} Z_{eff} &= \int \mathcal{D}\phi \exp \left( - \int K_S (\partial_\mu \phi)^2 + \right. \\ &\quad \left. \beta_S \int \cos\left(\frac{S}{\sqrt{2S}}(\varphi - \bar{\varphi})\right) + \right. \\ &\quad \left. \alpha_S \int \cos\left(\frac{2S}{\sqrt{2S}}(\varphi - \bar{\varphi})\right) + \dots \right), \end{aligned} \quad (22)$$

for  $S$  integer. Here the dots simply mean higher powers of the perturbing vertex operators and  $K_S$  is an effective constant arising from the OPE of vertex and parafermionic operators in the process of integration of the massive degrees of freedom. We immediately notice that for integer  $S$  there is an extra vertex operator coming from (19) which is not present for half-integer  $S$ , and as we will see, this difference between integer and half-integer effective actions is crucial.

Using (1) and (6) we can write the continuum expression of the original spin operator  $\vec{S}(x)$  as

$$\vec{S}(x) = \vec{J}_R + \vec{J}_L + (-1)^x \text{tr}(\vec{\sigma}/2(\Phi^{(1/2)} + \Phi^{(1/2)\dagger})). \quad (23)$$

One way to see whether the system is gapped or not is to study the behavior of the spin-spin correlation function at large scales. Since our original  $SU(2)$  WZW model is perturbed, correlation functions of the fundamental field will contain supplementary operators coming from the OPE between  $\Phi^{(1/2)}$  and the perturbing fields. With the help of the fusion rules

(14) it is easy to see that, for example, the effective alternating z-component of the spin operator containing the scalar field will be given by:

$$\sum_{k \leq 2S, k \text{ odd}} a_k \mu_k : e^{\frac{ik}{2\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c., \quad (24)$$

where only odd  $k$  fields appear in the sum. Let us consider now separately the case of half-integer and integer  $S$ : For  $S$  half-integer, the operator  $\Phi^{(S)}$  is present in (24), and we can easily check that, (since  $\mu_{2S}$  corresponds to the identity), this operator is simply given by

$$e^{\frac{iS}{\sqrt{2S}}(\varphi - \bar{\varphi})} + h.c.$$

The other operators in the series contain parafermionic disorder operators whose correlators will decay exponentially to zero at large scales. Thus, considering only the Gaussian part of (21), we can show that the spin correlation functions at large scales behave like:

$$\begin{aligned} \langle S_z(x) S_z(y) \rangle &\sim (-1)^{(x-y)} |x - y|^{-2SK_S} \\ \langle S_+(x) S_-(y) \rangle &\sim (-1)^{(x-y)} |x - y|^{-1/(2SK_S)} \end{aligned} \quad (25)$$

The fact that the  $SU(2)$  symmetry is unbroken at all scales fixes then the value of  $K_S$  to be

$$K_S = 1/(2S) \quad (26)$$

For this value of  $K_S$  one can show that the perturbing operator in (21) is marginally irrelevant.

We conclude then that the large scale behavior of half-integer spin chains is given by the level 1  $SU(2)$  WZW model with logarithmic corrections as for the spin 1/2 chain. An interesting extension of this analysis is to add an arbitrary dimerization to the chain. In the context of the WZW approach this corresponds to the addition of the field  $tr \Phi^{(1/2)} + h.c. \propto \mu_1 : e^{\frac{i}{2\sqrt{2S}}(\varphi(z) - \bar{\varphi}(\bar{z}))} : + h.c.$  in the perturbing terms [8]. Reproducing the same arguments as above, we see that this term has the effect of making the operator  $\cos(\frac{S}{\sqrt{2S}}(\varphi - \bar{\varphi}))$  appear in the effective action (21). Using (26), we see that now this operator is highly relevant and will so produce a gap in the excitation spectrum unless a fine tuning of the parameters is performed.

Let us consider now integer spins  $S$ . Since the series (24) for the effective spin operator contains only half-integer spins  $j$  (odd  $k$ 's), all the operators in the series will contain non-trivial parafermionic operators. Then all the terms in the spin-spin correlation function will decay exponentially to zero with the distance indicating the presence of a gap in the excitation spectrum, thus confirming Haldane's conjecture. This is our main result.

A possible modification consists in the addition of dimerization to the system (which again corresponds to the inclusion of the field  $tr \Phi^{(1/2)}$  as a perturbation). Then, also integer spin  $j$  terms (even  $k$ 's) will be generated (as indicated by the fusion rules (14)) in the effective spin operator and in particular the vertex operator (19) which is the only candidate for a power law decay of the spin-spin correlators. However, as for the (dimerized) half-integer spin case, the presence in (22) of the (relevant) first vertex operator prevent the system to be massless (this situation is similar to the one encountered in [19], in the context of abelian bosonization), indicating again that a fine tuning of the dimerization parameter has to be performed to get a massless regime.

We have presented the continuum limit of the spin- $S$  antiferromagnetic Heisenberg chain in terms of a parafermion Conformal Field Theory interacting with a compact  $U(1)$  boson. After integrating out the massive parafermions we have shown that HAF chains with half-odd-integer spins have a massless spectrum while those with integer spin have a gap to all excitations, in complete accordance with Haldane's conjecture.

It has been shown by using a mapping to the sigma model that a dimerized spin  $S$  chain should have  $2S + 1$  massless points in the dimerization parameter space [9]. This result was shown to be valid for large  $S$  and a detailed treatment of dimerization within the present approach could help to extend this result for small values of the spin.

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